Inverse design of porous materials using artificial neural networks

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Abstract

We have developed a user-desired generative adversarial network and used them to generate 121 zeolite materials. Generating optimal nanomaterials using artificial neural networks can potentially lead to a notable revolution in future materials design. Although progress has been made in creating small and simple molecules, complex materials such as crystalline porous materials have yet to be generated using any of the neural networks. Here, we have implemented a generative adversarial network that uses a training set of 31,713 known zeolites to produce 121 crystalline porous materials. Our neural network takes in inputs in the form of energy and material dimensions, and we show that zeolites with a user-desired range of 4 kJ/mol methane heat of adsorption can be reliably produced using our neural network. The fine-tuning of user-desired capability can potentially accelerate materials development as it demonstrates a successful case of inverse design of porous materials.